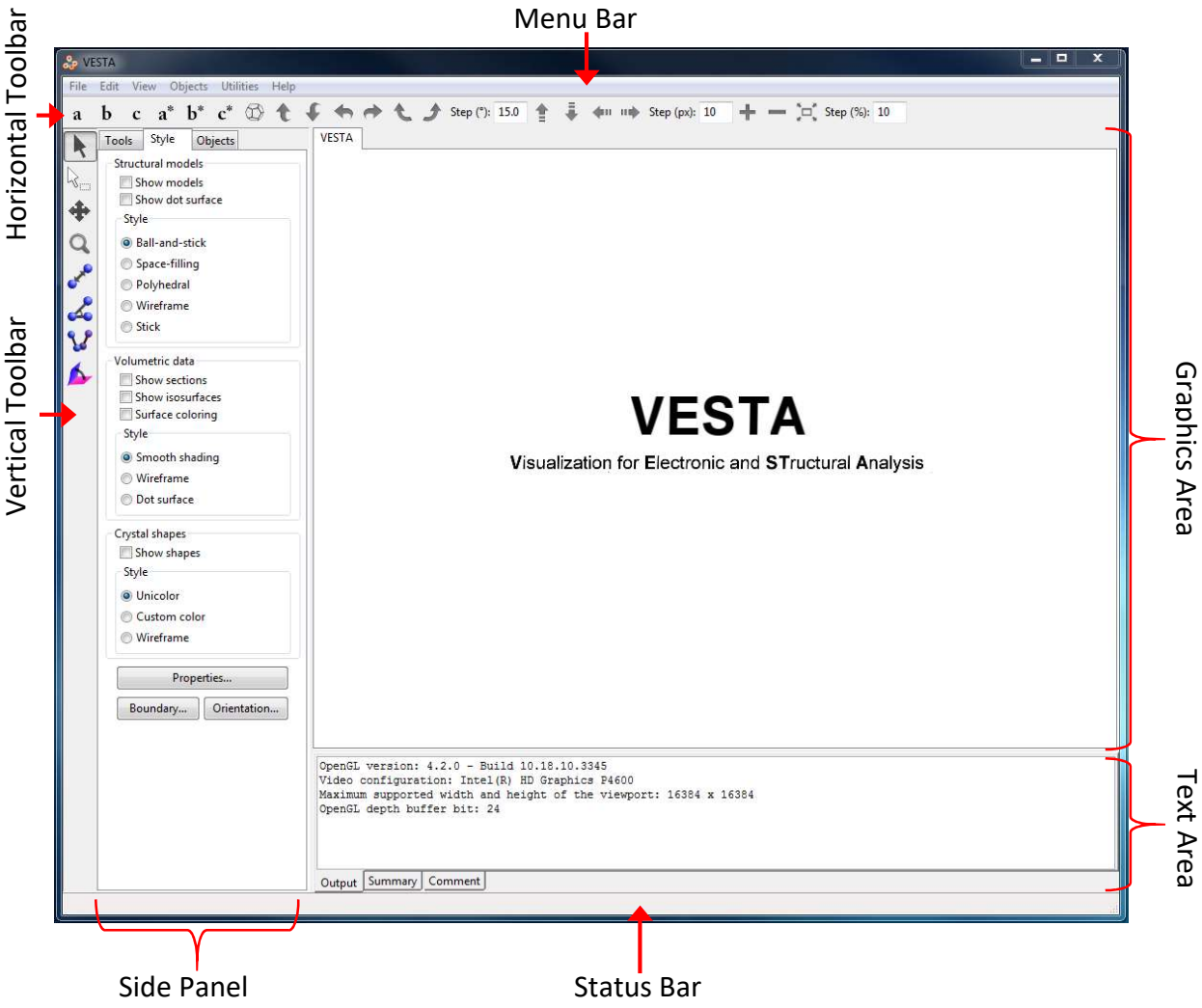
Exercise sheet 0

Introduction

1. Download (and run) the 3D visualization program VESTA from the web: http://jp-minerals.org/vesta/en/download.html
2. Make yourself familiar with the interface:



Exercise sheet 0A

Crystal structure of diamond and graphite.

1. Find and download the diamond and graphite VESTA files from: http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta_data

2. Open the downloaded files with VESTA (*File* → *Open*).

3. Display the unit cells for both structures by clicking on *Properties* in the *Style* tab of the side panel and choosing *Single unit cell* in the *General* tab of the opened window. Click *OK* to close the window.

4. For clarity, atoms outside of the unit cell can be omitted. Go to *Edit* → *Bonds*, select the 1st row of atoms (it should get highlighted in blue, orange, etc. depending on your OS) and change the *Boundary mode* to *Do not search atoms beyond the boundary*. Click *OK* to close the window.

5. Rotate (click and hold left while moving the cursor) and translate (choose *Translate* mode  from the vertical toolbar and click and hold left while moving the cursor) the displayed structure. If you go to the side panel and select the *Tools* tab, you can choose to only rotate around the X, Y or Z axis. You can zoom using the mouse wheel or the *Zoom in* / *Zoom out* buttons  in the horizontal toolbar. The original orientation can be restored by clicking on the *Standard orientation of crystal shape* button  and the *Fit to the screen* button  .

6. What atoms are diamond and graphite made of? You can use the *Select* mode  from the vertical toolbar, click on an atom and see its species, coordinates and other information in the *Output* tab of the text area.

7. Change the number of displayed unit cells. In the side panel choose the *Style* tab, click on *Boundary* and change x(max), y(max) and z(max) at will. (Warning: Displaying a large number of atoms can slow down the program significantly.)

8. What are qualitative differences between the two crystal structures?

9. What is the shortest distance between two atoms in diamond and graphite? Use the *Distance* tool  from the vertical toolbar and click on two atoms one after the other. The corresponding distance can be seen in the *Output* tab of the text area.

Exercise sheet 0B

Crystal structure of diamond and boron-nitride (cubic).

1. Find and download the diamond and cubic boron-nitride (BN) VESTA files from: http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta_data

2. Open the downloaded files with VESTA, display the unit cell and omit all atoms outside of it.

3. For boron-nitride, try different display styles (*ball-and-stick*, *Space-filling*, etc.) in the *Style* tab of the side panel.

4. Open again *Properties*. In the *Atoms* tab you can change the *Radii type*. Try different types.

5. What is the shortest distance between two atoms in boron-nitride?

6. Determine the B-N-B bond angle using an appropriate tool.

7. Are the crystal structures of diamond and boron-nitride the same? If not, what are the differences? What are the underlying lattices?

8. What material properties do diamond and boron-nitride have in common? (Feel free to use the Internet / library.)

Exercise sheet 0C

Crystal structure of gold.

1. Find and download the gold (Au) VESTA file from:
   http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta_data

2. Open the downloaded file with VESTA, display the unit cell and omit all atoms outside of it.

3. The program does not draw any connections between the atoms. What might be the reason for this?

4. What is the distance between nearest and next-nearest neighbours?

5. Look up the mass of a gold atom and calculate the mass-density of gold. (Think carefully about how many atoms there are per unit cell!)

Exercise sheet 0D

Crystal structure of iron and table salt (NaCl)

1. Find and download the iron (Fe) and NaCl VESTA files from:
   http://www.misasa.okayama-u.ac.jp/~masami/pukiwiki/index.php?Vesta_data
   (There are two files for iron. Download both of them.)

2. Try to find out why there are two files available for iron (Fe-bcc and Fe-fcc).

3. Open the downloaded files with VESTA, display the unit cell and omit all atoms outside of it.

4. Which of the two (Fe-bcc or Fe-fcc) has the same underlying lattice as NaCl? You can hide atoms by selecting them and pressing *Del*. Pressing *Esc* makes them reappear.

5. Calculate the density of bcc iron and NaCl and compare it to the one of gold.